

# Level spacings at the metal-insulator transition in the Anderson Hamiltonians and multifractal random matrix ensembles

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We consider orthogonal, unitary, and symplectic ensembles of random matrices with  $(1/a)(\ln x)^2$  potentials, which obey spectral statistics different from the Wigner-Dyson and are argued to have multifractal eigenstates. If the coefficient  $a$  is small, spectral correlations in the bulk are universally governed by a translationally invariant, one-parameter generalization of the sine kernel. We provide analytic expressions for the level spacing distribution functions of this kernel, which are hybrids of the Wigner-Dyson and Poisson distributions. By tuning the single parameter, our results can be excellently fitted to the numerical data for three symmetry classes of the three-dimensional Anderson Hamiltonians at the metal-insulator transition, previously measured by several groups using exact diagonalization.

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## I. INTRODUCTION

Quantum mechanics described by stochastic ensembles of Hamiltonians [1], and by Hamiltonians with classically chaotic trajectories [2], have been a subject of intense study for years. In contrast to Hamiltonians of classically integrable systems whose energy levels are mutually uncorrelated, chaotic Hamiltonians generally exhibit strong correlation among levels. To simulate this level repulsion in chaotic or disordered Hamiltonians, Wigner introduced the random matrix ensembles (RME) [3]. In the RME defined as an integral over  $N \times N$  matrices, only the antiunitary symmetry of the Hamiltonian is respected, and its spatial structure is completely discarded. Despite this extreme idealization, analytic predictions from RME's beautifully explain the spectral statistics of chaotic or disordered Hamiltonians [4]. This success is accounted for by the fact that the RME is not merely an idealization of disordered Hamiltonians but it is indeed equivalent to the latter under a situation where the mean energy level spacing  $\Delta$  is much smaller than the Thouless energy  $E_c$  (inverse classical diffusion time) that the dimensionality does become unimportant [5]. This on the other hand implies that in a region where the mean level spacing is equal to or larger than the Thouless energy, and the associated states tends to localize due to diffusion, standard RME's cannot provide good quantitative descriptions.

As a concrete example of systems of disordered conductors, let us take the Anderson tight-binding Hamiltonian (AH) [6,7],

$$H = \sum_{\mathbf{r}} \varepsilon_{\mathbf{r}} a_{\mathbf{r}}^\dagger a_{\mathbf{r}} + \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} a_{\mathbf{r}}^\dagger a_{\mathbf{r}'}, \quad (1)$$

describing free electrons in a random potential. Here  $a_{\mathbf{r}}^\dagger$  and  $a_{\mathbf{r}}$  are creation and annihilation operators of an electron at a site  $\mathbf{r}$  on a three-dimensional (3D) toroidal lattice of size  $L^3$ ,  $\varepsilon_{\mathbf{r}}$ 's are site energies that are mutually

independent stochastic variables derived from a uniform distribution on an interval  $[-W/2, W/2]$ , and the sum  $\langle \mathbf{r}, \mathbf{r}' \rangle$  is over all pairs of nearest-neighboring sites. The antiunitary symmetry of the AH [Eq. (1)] is orthogonal ( $\beta = 1$ ), as it respects the time-reversal symmetry and has no spin dependence. For small values of disorder  $W$ , all eigenstates are extended. An overlap of such extended states  $\Psi_i(\mathbf{r})$  and  $\Psi_j(\mathbf{r})$  is expected to induce repulsion between associated eigenvalues, of the form  $|x_i - x_j|$ . Then the statistical fluctuation of these eigenvalues is described well by the Gaussian orthogonal ensemble of random matrices whose joint probability distribution consists of the product of a Vandermonde determinant  $\prod_{i < j} |x_i - x_j|$  and Gaussian factors  $\prod_i e^{-x_i^2}$ . The quadratic potential in the latter is merely for the sake of technical simplicity, and the deformation of the potential by generic polynomials universally leads to the same Wigner-Dyson statistics [8]. As we increase the disorder  $W$ , states associated with eigenvalues close to the edges of the spectral band are believed to start localizing. When the disorder is as large as to induce the metal-insulator transition (MIT)  $E_c/\Delta \simeq 1$ , eigenstates are observed to be multifractal [9], characterized by an anomalous scaling behavior of the moments of inverse participation ratio [10–12]

$$\sum_{\mathbf{r}} \langle |\Psi_i(\mathbf{r})|^{2p} \rangle \propto L^{-D_p(p-1)}. \quad (2)$$

This property implies a slowly decreasing overlap between states [13] (for  $|x_i - x_j| \gg \Delta$ ),

$$\sum_{\mathbf{r}} \langle |\Psi_i(\mathbf{r})|^2 |\Psi_j(\mathbf{r})|^2 \rangle \propto |x_i - x_j|^{-(1-D_2/d)}. \quad (3)$$

For large enough disorder, the off-diagonal (hopping) term of the AH becomes negligible, leading to mutually uncorrelated eigenvalues. Each eigenstate is almost localized to a single site. Thus the spectrum of the AH shows a gradual crossover from the Wigner-Dyson to the Poisson

as one increases the disorder  $W$ , while keeping the size  $L$  fixed finite. A characteristic observable in these studies of spectral statistics is the probability  $E(s)$  of having no eigenvalue in an interval of width  $s$ , or equivalently the probability distribution of spacings of two consecutive eigenvalues  $P(s) = E''(s)$ . These observables capture the behavior of local correlations of a large number of energy eigenvalues, as the former consists of an infinite sum of integrals of regulated spectral correlators (the subscript  $\text{reg}$  denotes its regular part, i.e., with  $\delta$ -functional peaks at coincident  $x_i$ 's subtracted),

$$E(s) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{-s/2}^{s/2} dx_1 \cdots dx_n \langle \rho(x_1) \cdots \rho(x_n) \rangle_{\text{reg}}, \quad (4)$$

and are more conveniently measured by the exact diagonalization of random Hamiltonians than the spectral correlators. The Poisson distribution is characterized by  $P_{\text{P}}(s) = \exp(-s)$ , and the Wigner-Dyson distribution is well approximated by the Wigner surmise  $P_{\text{W}}(s) = (\pi s/2) \exp(-\pi s^2/4)$ .

Recent technical developments [14–26] on the exact diagonalization of the AH on a large size of lattices prompted analytical studies on its spectrum [27–31]. It was noticed in Ref. [14] that at the MIT point with disorder  $W \sim 16.5$ , the level spacing distribution function (LSDF)  $P(s)$  is independent of the size  $L$ . From this finding these authors have argued that in the thermodynamic limit there exist only three universality classes: Wigner-Dyson, Poisson, and the third, critical statistics. The presence of critical LSDF's was also observed for the unitary ( $\beta = 2$ ) and symplectic ( $\beta = 4$ ) cousins, i.e., AH's under a magnetic field [18,20,24],

$$H = \sum_{\mathbf{r}} \varepsilon_{\mathbf{r}} a_{\mathbf{r}}^\dagger a_{\mathbf{r}} + \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} V_{\mathbf{r}\mathbf{r}'} a_{\mathbf{r}}^\dagger a_{\mathbf{r}'}, \quad (5)$$

$$V_{\mathbf{r}, \mathbf{r} \pm \hat{\mathbf{x}}} = e^{\mp 2\pi i \alpha r_y}, \quad V_{\mathbf{r}, \mathbf{r} \pm \hat{\mathbf{y}}} = V_{\mathbf{r}, \mathbf{r} \pm \hat{\mathbf{z}}} = 1,$$

and with spin-orbit coupling [16,25,21],

$$H = \sum_{\mathbf{r}, \sigma=\pm} \varepsilon_{\mathbf{r}} a_{\mathbf{r}\sigma}^\dagger a_{\mathbf{r}\sigma} + \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma, \sigma'} V_{\mathbf{r}\sigma, \mathbf{r}'\sigma'} a_{\mathbf{r}\sigma}^\dagger a_{\mathbf{r}'\sigma'}, \quad (6)$$

$$V_{\mathbf{r}\sigma, \mathbf{r} \pm \hat{\mathbf{i}}\sigma'} = (e^{\mp i\theta\sigma_i})_{\sigma\sigma'} \quad (\hat{\mathbf{i}} = \hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}).$$

The critical LSDF's are found to be independent of the strength of the magnetic field  $\alpha$  or the spin-orbit coupling  $\theta$ . For all values of  $\beta$ , the Wigner-Dyson-like behaviors  $P_{(\text{cr})}(s) \propto s^\beta$  for small  $s$  have been confirmed. There were disputes over the large  $s$  asymptotic behavior of the LSDF's, but accurate measurements on large lattices [23] strongly support the Poisson-like behavior  $P_{(\text{cr})}(s) \sim \exp(-\text{const} \times s)$  for large  $s$ , excluding a non-trivial exponent  $P_{(\text{cr})}(s) \sim \exp(-\text{const} \times s^{1+\gamma})$  predicted in Ref. [29]. In the light of the success of the random matrix (RM) description of extended states, a natural resort to describe this critical statistics is to consider a deformed RME that violates the above mentioned universality of

the Wigner-Dyson statistics for the Gaussian ensembles. The validity of the RM description for such critical systems is of course far from clear, because the existence of the MIT crucially relies upon the dimensionality, whereas the RME has no spatial structure. Nevertheless, under an assumption that the spectra of the AH be described by RME's, an attempt [32] was made to reconstruct a random matrix potential out of the macroscopic spectra of the AH. There, it was observed that a potential of the form

$$V(x) = \frac{1}{2a} [\ln(1 + b|x|)]^2 \quad (7)$$

explains well the numerical data. The above potential indeed violates the universality of the Wigner-Dyson statistics that is guaranteed only for polynomial potentials [33]. This observation leads to a speculation that the critical level spacing distribution might be derived from a RME with a potential (7). Later the LSDF of orthogonal RME's of type (7) has been measured by using the Monte Carlo simulation [34] in order to compare it with that from exact diagonalization of the AH [22]. Excellent agreement between the two was found by tuning the parameter  $a$  to 2.5. Motivated by this success, we shall derive analytic forms of the LSDF's of RME's with orthogonal, unitary and symplectic symmetries. (The unitary case has already been reported [35].) In doing so, we shall retain all perturbative (polynomial in  $a$ ) parts of the spectral kernel, and discard unphysical nontranslationally invariant parts of order  $O(e^{-\pi^2/a})$ .

This paper is organized as follows. In Sec. II we review nonstandard features of RME's with log-squared potentials. In Sec. III we follow the method of Tracy and Widom [47] to derive the LSDF's from an approximated translationally invariant kernel. In Sec. IV we shall compare our results with the numerical data of the AH's with orthogonal, unitary, and symplectic symmetries. In Appendix A we collect standard results on Fredholm determinants in random matrix theories that are relevant for our purpose.

## II. RME WITH LOG-SQUARED POTENTIAL

In this section we review properties of RME's with log-squared potentials. For small enough  $a$ , we derive a translationally invariant kernel, whose level spacing distribution will be our subject in this paper.

We consider  $N \times N$  random real symmetric ( $\beta = 1$ ), complex hermitian ( $\beta = 2$ ), and quaternion selfdual ( $\beta = 4$ ) matrix ensembles, whose joint probability densities of eigenvalues are given by

$$\mathcal{P}_\beta(\lambda_1, \dots, \lambda_N) \propto \prod_{i=1}^N e^{-V(\lambda_i)} \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^\beta. \quad (8)$$

with a potential growing as

$$V(\lambda) \sim \frac{1}{2a} (\ln \lambda)^2 \quad (\lambda \gg 1). \quad (9)$$

The potential is assumed to be regularized at the origin, as in Eq. (7). For a particular form of the potential

$$V(\lambda) = \sum_{n=1}^{\infty} \ln[1 + 2q^n \cosh(2 \operatorname{arcsinh}\lambda) + q^{2n}], \quad (10)$$

( $0 < q < 1$ ), which behaves as Eq. (9) with  $a = \ln(1/q)/2$ , corresponding orthogonal polynomials are known as the  $q$ -Hermite polynomials [36]. Using their asymptotic form, Muttalib *et al.* [37] have obtained the exact kernel for the unitary ensemble with the potential (10) in the large  $N$  limit,

$$K^{(\text{exact})}(x, y) = \text{const} \times \frac{\sqrt{\cosh 2ax \cosh 2ay}}{\cosh a(x+y)} \times \frac{\vartheta_4(x+y, e^{-\pi^2/a})}{\sqrt{\vartheta_4(2x, e^{-\pi^2/a})\vartheta_4(2y, e^{-\pi^2/a})}} \frac{\vartheta_1(x-y, e^{-\pi^2/a})}{\sinh a(x-y)}. \quad (11)$$

Here  $\vartheta_\nu$  are the elliptic theta functions, and the variable  $x \equiv \lambda/(2a)$  is so rescaled that the average level spacing is unity. In order to eliminate nonuniversal effects involved by the regularization of the potential in the vicinity of the origin from the bulk correlation, we need to take

$$x, y \gg 1, \quad \text{with } |x-y| = \text{bounded}. \quad (12)$$

Then we obtain an asymptotic form of the kernel

$$K^{(\text{asympt})}(x, y) = \text{const} \times \frac{\vartheta_4(x+y, e^{-\pi^2/a})}{\sqrt{\vartheta_4(2x, e^{-\pi^2/a})\vartheta_4(2y, e^{-\pi^2/a})}} \frac{\vartheta_1(x-y, e^{-\pi^2/a})}{\sinh a(x-y)}. \quad (13)$$

The above kernel is still not translationally invariant due to the reason explained below. Now we make a further simplification of the kernel by using an approximation. For  $e^{-\pi^2/a} \ll 1$ , we can discard subleading orders from the  $q$  expansion of the theta functions in terms of trigonometric functions. Then we obtain a translationally invariant kernel, up to  $O(e^{-\pi^2/a})$ ,

$$K(x, y) = \frac{a}{\pi} \frac{\sin \pi(x-y)}{\sinh a(x-y)}. \quad (14)$$

The universality of this deformed kernel within RME's is observed for the  $q$ -Laguerre unitary ensemble [38], the finite-temperature Fermi gas model [39], and subsequently for unitary ensembles whose potentials have the asymptotics (9) [34]. This universality can be considered as an extension of the universality of the sine kernel [8],

$$K(x, y) = \frac{\sin \pi(x-y)}{\pi(x-y)}, \quad (15)$$

for polynomially increasing potentials, proven via the asymptotic WKB form of the wave functions

$$\psi_N(\lambda) \sim \cos \left( \pi \int^\lambda \rho(\lambda) d\lambda + \frac{N\pi}{2} \right), \quad (16)$$

$$K(\lambda, \lambda') \sim \frac{\sin[\pi(\int^\lambda \rho - \int^{\lambda'} \rho)]}{\lambda - \lambda'}. \quad (17)$$

Here  $\rho(\lambda)$  stands for the exact unnormalized spectral density,  $K(\lambda, \lambda')$ . In the spectral bulk of the RME with polynomially increasing potentials, the spectral density divided by  $N$  is bounded, and is locally approximated by a constant when measuring  $\lambda$  in unit of the mean level spacing. This slowly-varying function is called the mean-field spectral density  $\bar{\rho}(\lambda)$ , given by [40]

$$\bar{\rho}(\lambda) \equiv \frac{N}{\pi\sqrt{R^2 - \lambda^2}} + \frac{1}{\pi^2} \int_{-R}^R \frac{d\mu}{\lambda - \mu} \sqrt{\frac{R^2 - \lambda^2}{R^2 - \mu^2}} \frac{V'(\mu)}{2}. \quad (18)$$

Here  $\pm R$  are the end points of the spectrum, determined by  $\int_{-R}^R \bar{\rho}(\lambda) d\lambda = N$ . After replacing the exact  $\rho(\lambda)$  by the mean-field  $\bar{\rho}(\lambda)$ , the unfolding map

$$\lambda \mapsto x = \int^\lambda \bar{\rho}(\lambda) d\lambda \quad (19)$$

becomes merely a linear transformation, leading universally to the sine kernel. On the other hand, in our case of the potential (9), the mean-field spectral density (18) behaves as

$$\bar{\rho}(\lambda) \sim \frac{1}{2a|\lambda|}, \quad (20)$$

implying an unusual unfolding map

$$\lambda \mapsto x = \frac{1}{2a} \operatorname{sgn}(\lambda) \ln |\lambda|, \quad (21)$$

while the formula (17) stays valid [41]. Then the kernel (17) universally reduces to Eq. (14) after this unfolding.

It is clear from the form of the kernel (14) that a set of eigenvalues with  $|x_i - x_j| \gg 1/a$  obeys the Poisson statistics, i.e., is uncorrelated. On the other hand, a set of eigenvalues with  $|x_i - x_j| \ll 1/a$  obeys the Wigner-Dyson statistics, because Eq. (14) is then approximated by the sine kernel, up to  $O(a^2)$ . To be precise, the kernel (14) signifies the multifractality of the eigenstates [42]. To see this, we first note that the property (3) of the fractal states leads to a compressible gas of eigenvalues, i.e., a linear asymptotics of the number variance  $\Sigma^2$  within an energy window of width  $S$  [43] [ $Y_2(x) \equiv 1 - \langle \rho(x)\rho(0) \rangle_{\text{reg}}$ ],

$$\Sigma^2(S) \equiv S - 2 \int_0^S dx (S-x) Y_2(x) \quad (22)$$

$$\sim \frac{1}{2} \left( 1 - \frac{D_2}{d} \right) S \equiv \chi S \quad (S \gg 1). \quad (23)$$

The RME's with the scalar kernel (14) indeed enjoy this asymptotic behavior with the level compressibility  $\chi$  given by

$$\chi = \frac{a}{\pi^2} + O(e^{-2\pi^2/a}) \quad (24)$$

for unitary [38,42] and orthogonal ensembles, and for the symplectic ensemble the exponential correction is replaced by  $O(e^{-\pi^2/a})$ . Moreover, the *multiplicity* of the RME's with the deformed kernel (14) has been concluded [42] through the equivalence between the finite-temperature Fermi gas model (having the universal deformed kernel) and a Gaussian banded RME that is proven to have multifractal eigenstates [44]. This brings forth the possibility of describing the spectral statistics of the AH's at the MIT by RME's with the deformed kernel.

We should emphasize an important fact that the RME's with log-squared potentials cannot describe disordered systems with large disorder. While the AH in the  $W \rightarrow \infty$  limit leads to the Poisson statistics, the RME with Eq. (9) does not obey the Poisson statistics in the limit  $a \rightarrow \infty$  [34,45]. It is because the joint probability distribution of RME's after the unfolding (21) leads to

$$\begin{aligned} \mathcal{P}_\beta(x_1, \dots, x_N) &= \text{const} \times \\ &\prod_{1 \leq i < j \leq N} \left| \pm e^{2a|x_i|} \mp e^{2a|x_j|} \right|^\beta \prod_{i=1}^N e^{-2ax_i^2} e^{2a|x_i|}. \end{aligned} \quad (25)$$

In the limit  $a \rightarrow \infty$ , each factor of  $|e^{2a|x_i|} \mp e^{2a|x_j|}|^\beta$  is dominated by an exponential with a larger modulus. Thus the Vandermonde determinant is approximated by

$$\prod_{i=1}^N e^{2a\beta(i-1)|x_i|} \quad (\text{for } |x_1| < \dots < |x_N|). \quad (26)$$

Consequently  $\mathcal{P}_\beta(x_1, \dots, x_N)$  tends to a product of very narrow [of variance  $\sigma^2 = 1/(4a\beta) \ll 1$ ] Gaussian distributions obeyed by  $x_i$  whose center is at  $[\beta(i-1) + 1]/2$ . This “crystallization” of eigenvalues invalidates naively expected mutual independence of distributions of eigenvalues, and drives the spectrum toward an exotic statistics different from Poissonian [45]. This phenomenon can be rephrased in the context of using the WKB formula (17) to derive the kernel (14). Although Eq. (17) remains valid even in the case  $a \rightarrow \infty$ , use of the mean-field spectral density  $\bar{\rho}(\lambda) = 1/(2a\lambda)$  in place of the exact  $\rho(\lambda)$  is not justifiable, because the crystallization of eigenvalues leads to a rapidly oscillating  $\rho(\lambda)$ . In the case of the  $q$ -Hermite ensemble (10), the potential itself has a oscillation of the same type, leading again to crystallization [45]. Therefore, the RME with log-squared potentials, despite the fact that it is constructed from the macroscopic spectra of the AH, should be considered as a good model of the latter only for small values of  $a$  where the

level repulsion property of the Gaussian ensembles is deformed slightly but not to the extent that the crystallization of eigenvalues becomes prominent. In the case of the  $q$ -Hermite ensembles, we can estimate this scale to be characterized by the value of  $a$  where nontranslational invariance of the exact kernel becomes manifest, i.e.,  $e^{-\pi^2/a} \simeq 1$ . We assume this estimate to be valid generically for RME's with log-squared potentials (9). In view of this, for our purpose of reproducing the LSDF of the AH, we shall concentrate on the approximated universal kernel (14). This will be justified *a posteriori*, after confirming that the best-fit value of the parameter  $a$  for the MIT point of the AH's are such that  $e^{-\pi^2/a} \ll 1$ .

### III. LEVEL SPACING DISTRIBUTIONS OF THE DEFORMED KERNEL

In this section we analytically compute the LSDF  $P_\beta(s)$  from the deformed kernel (14) for all values of the Dyson index  $\beta$ . Our result completes earlier attempts to compute  $P_2(s)$  numerically [37] or asymptotically [46], and is consistent with those.

We notice that the kernel (14) is equivalent to that of Dyson's circular unitary ensemble at finite  $N$  [3],

$$K(x, y) = \frac{\sin(N/2)(x-y)}{N \sin(1/2)(x-y)}, \quad (27)$$

by the following analytic continuation

$$N \rightarrow \frac{\pi i}{a}, \quad x \rightarrow \frac{2a}{i}x. \quad (28)$$

Tracy and Widom [47] have proven that the diagonal resolvent kernel of Eq. (27) is determined by a second-order differential equation that is reduced to a Painlevé VI equation [48]. We shall follow their method below.

The kernel (14) is written as

$$\begin{aligned} K(x, y) &= \frac{\phi(x)\psi(y) - \psi(x)\phi(y)}{e^{2ax} - e^{2ay}}, \\ \phi(x) &= \sqrt{\frac{2a}{\pi}} e^{ax} \sin \pi x, \quad \psi(x) = \sqrt{\frac{2a}{\pi}} e^{ax} \cos \pi x. \end{aligned} \quad (29)$$

These component functions satisfy

$$\phi' = a\phi + \pi\psi, \quad \psi' = -\pi\phi + a\psi. \quad (30)$$

We use the bra-ket notation  $\phi(x) = \langle x|\phi\rangle$  and so forth [50]. Due to our choice of the component functions to be real valued (unlike [47], Sec. V D), we have  $\langle x|O|\phi\rangle = \langle \phi|O|x\rangle$  and a similar situation for  $\psi$  with any self-adjoint operator  $O$  and real  $x$ . Then Eq. (29) is equivalent to

$$[e^{2aX}, K] = |\phi\rangle\langle\psi| - |\psi\rangle\langle\phi|, \quad (31)$$

where  $X$  and  $K$  are the multiplication operator of the independent variable and the integral operator with the kernel  $K(x, y)\theta(y-t_1)\theta(t_2-y)$ , respectively. Below we

will not explicitly write the dependence on the end points of the underlying interval  $[t_1, t_2]$ . It follows from Eq. (31) that

$$\left[ e^{2ax}, \frac{K}{1-K} \right] = \frac{1}{1-K} (|\phi\rangle\langle\psi| - |\psi\rangle\langle\phi|) \frac{1}{1-K}, \quad (32)$$

that is,

$$\begin{aligned} (e^{2ax} - e^{2ay})R(x, y) &= Q(x)P(y) - P(x)Q(y), \\ Q(x) &\equiv \langle x | (1-K)^{-1} |\phi\rangle, \\ P(x) &\equiv \langle x | (1-K)^{-1} |\psi\rangle. \end{aligned} \quad (33)$$

At a coincident point  $x = y$  we have

$$2a e^{2ax} R(x, x) = Q'(x)P(x) - P'(x)Q(x). \quad (34)$$

Now, by using the identity

$$\frac{\partial K}{\partial t_i} = (-1)^i K |t_i\rangle\langle t_i| \quad (i = 1, 2), \quad (35)$$

we obtain

$$\frac{\partial Q(x)}{\partial t_i} = (-1)^i R(x, t_i)Q(t_i), \quad (36a)$$

$$\frac{\partial P(x)}{\partial t_i} = (-1)^i R(x, t_i)P(t_i). \quad (36b)$$

On the other hand, by using the identity ( $D$  is the derivation operator)

$$[D, K] = K(|t_1\rangle\langle t_1| - |t_2\rangle\langle t_2|), \quad (37)$$

which follows from the translational invariance of the kernel  $(\partial_x + \partial_y)K(x - y) = 0$ , we also have

$$\begin{aligned} \frac{\partial Q(x)}{\partial x} &= \langle x | D(1-K)^{-1} |\phi\rangle \\ &= \langle x | (1-K)^{-1} |\phi'\rangle \\ &\quad + \langle x | (1-K)^{-1} [D, K](I-K)^{-1} |\phi\rangle \\ &= aQ(x) + \pi P(x) + R(x, t_1)Q(t_1) - R(x, t_2)Q(t_2), \end{aligned} \quad (38a)$$

$$\begin{aligned} \frac{\partial P(x)}{\partial x} &= -\pi Q(x) + aP(x) + R(x, t_1)P(t_1) - R(x, t_2)P(t_2). \end{aligned} \quad (38b)$$

Now we set  $t_1 = -t$ ,  $t_2 = t$ ,  $x, y = -t$  or  $t$ , and introduce notations  $\tilde{q} = Q(-t)$ ,  $q = Q(t)$ ,  $\tilde{p} = P(-t)$ ,  $p = P(t)$ , and  $\tilde{R} = R(-t, t) = R(t, -t)$ ,  $R = R(t, t) = R(-t, -t)$ . The last two equalities follow from the evenness of the kernel. Then Eqs. (33) and (34) read, after using Eqs. (38),

$$\tilde{p}q - \tilde{q}p = 2\tilde{R} \sinh 2at, \quad (39a)$$

$$\tilde{p}^2 + \tilde{q}^2 = \frac{2}{\pi} (\tilde{R}^2 \sinh 2at + Ra e^{-2at}), \quad (39b)$$

$$p^2 + q^2 = \frac{2}{\pi} (\tilde{R}^2 \sinh 2at + Ra e^{2at}). \quad (39c)$$

The total  $t$  derivatives of Eqs. (39) lead to ( $\cdot = d/dt$ )

$$\tilde{p}\tilde{p} + \tilde{q}\tilde{q} = \frac{1}{\pi} (\tilde{R} \sinh 2at), \quad (40)$$

$$\dot{R} = 2\tilde{R}^2, \quad \ddot{R} = 4\tilde{R}\dot{\tilde{R}}. \quad (41)$$

The left-hand sides of Eqs. (39) and (40) satisfy an additional constraint,

$$(\tilde{p}\tilde{p} + \tilde{q}\tilde{q})^2 + (\tilde{p}\tilde{q} - \tilde{q}\tilde{p})^2 = (\tilde{p}^2 + \tilde{q}^2)(p^2 + q^2). \quad (42)$$

By eliminating  $\tilde{p}$ ,  $p$ ,  $\tilde{q}$ ,  $q$ ,  $\tilde{R}$ , and  $\dot{\tilde{R}}$  from Eqs. (39)–(42), we obtain for  $R(s)$  ( $s \equiv 2t$ ,  $' = d/ds$ )

$$\begin{aligned} &\left[ a \cosh as R'(s) + \frac{\sinh as}{2} R''(s) \right]^2 + [\pi \sinh as R'(s)]^2 = \\ &R'(s) ([aR(s)]^2 + a \sinh 2as R(s) R'(s) + [\sinh as R'(s)]^2). \end{aligned} \quad (43)$$

It is equivalent to Eq. (5.70) of Ref. [47] after the analytic continuation (28), accompanied by a redefinition  $R(s) \rightarrow (i/2a)R(s)$ . This is slightly nontrivial because Ref. [47] has used  $\tilde{p} = p^*$  and  $\tilde{q} = q^*$ , which follow from the analytic properties of its component functions,  $\phi(-x) = \phi(x)^*$  and  $\psi(-x) = \psi(x)^*$ . In the limit  $a \rightarrow 0$ , it clearly reduces to the  $\sigma$  form of a Painlevé V equation

$$\left[ R'(s) + \frac{s}{2} R''(s) \right]^2 + [\pi s R'(s)]^2 = R'(s) [R(s) + s R'(s)]^2, \quad (44)$$

derived for the sine kernel (15) of the Gaussian ensembles [49]. Note that for  $\beta = 1$ , a replacement  $a \rightarrow a/2$  is necessary because of our convention (A1).

Finally, the LSDF's  $P_\beta(s)$  are expressed in terms of the diagonal resolvent  $R(s)$  via Eqs. (A12), (A14), and the first of Eq. (41):

$$P_1(s) = \left[ e^{-\frac{1}{2} \int_0^s ds [R(s) + \sqrt{R'(s)}]} \right]'' , \quad (45a)$$

$$P_2(s) = \left[ e^{-\int_0^s ds R(s)} \right]'' , \quad (45b)$$

$$P_4(s) = \left[ e^{-\frac{1}{2} \int_0^{2s} ds R(s)} \cosh \left( \frac{1}{2} \int_0^{2s} ds \sqrt{R'(s)} \right) \right]'' . \quad (45c)$$

The boundary condition follows from the expansion (4) of  $E_2(s)$  in terms of the correlation functions:

$$\begin{aligned} E_2(s) &= 1 - \int_{-s/2}^{s/2} dx K(x, x) \\ &\quad + \frac{1}{2} \int_{-s/2}^{s/2} dx_1 dx_2 \det_{i,j=1,2} K(x_i, x_j) - \dots \\ &= 1 - s + O(s^4), \end{aligned} \quad (46)$$

$$R(s) = -[\ln E_2(s)]' = 1 + s + \dots \quad (47)$$

Our main result consists of Eqs. (43), (45), and (47).

For  $s \ll 1/a$ , we can Taylor-expand hyperbolic functions, to obtain a perturbative solution to Eq. (43),

$$R(s) = 1 + s + s^2 + \left(1 - \frac{\pi^2 + a^2}{9}\right)s^3 + \left(1 - \frac{5(\pi^2 + a^2)}{36}\right)s^4 + \left(1 - \frac{(\pi^2 + a^2)(75 - 4\pi^2 - 6a^2)}{450}\right)s^5 + \dots, \quad (48)$$

$$\begin{aligned} P_1(s) &= \frac{4\pi^2 + a^2}{24}s - \frac{(4\pi^2 + a^2)(12\pi^2 + 7a^2)}{2880}s^3 + \frac{(\pi^2 + a^2)(4\pi^2 + a^2)}{1080}s^4 \\ &\quad + \frac{(4\pi^2 + a^2)(48\pi^4 + 72\pi^2a^2 + 31a^4)}{322560}s^5 - \frac{(\pi^2 + a^2)(4\pi^2 + a^2)(12\pi^2 + 13a^2)}{226800}s^6 + \dots, \end{aligned} \quad (49a)$$

$$P_2(s) = \frac{\pi^2 + a^2}{3}s^2 - \frac{(\pi^2 + a^2)(2\pi^2 + 3a^2)}{45}s^4 + \frac{(\pi^2 + a^2)(\pi^2 + 2a^2)(3\pi^2 + 5a^2)}{945}s^6 + \dots, \quad (49b)$$

$$P_4(s) = \frac{16(\pi^2 + a^2)(\pi^2 + 4a^2)}{135}s^4 - \frac{128(\pi^2 + a^2)(\pi^2 + 4a^2)(3\pi^2 + 13a^2)}{14175}s^6 + \dots. \quad (49c)$$

The above perturbative expansions are correct for the kernel (13) of the  $q$ -Hermite ensemble in any polynomial orders of  $a$ , while they lack nonperturbative terms of order  $e^{-\pi^2/a}$ , which depend on the reference point. On the other hand, for  $s \gg 1/a$ , it can be proven from Eq. (43) that  $R(s)$  approaches a constant. Then Eqs. (45) imply

$$\ln P_1(s) \sim -\frac{1}{2}R_{\frac{a}{2}}(\infty)s, \quad (50a)$$

$$\ln P_{2,4}(s) \sim -R_a(\infty)s, \quad (50b)$$

for  $s \rightarrow \infty$ . In Fig. 1 we exhibit the decay rate  $\kappa(a) \equiv R_a(s = \infty)$  for  $0 < a < 4$  computed numerically from Eq. (43). At present we could not find an analytic form of  $\kappa(a)$ . For small  $a (< 0.5)$ , it is well approximated by  $1/\kappa(a) \approx 0.202a$ , which agrees extremely well with the value  $2/\pi^2 = 0.2028$  expected from Eq. (24) and the analytic formula [27] that holds in generality,

$$\chi = \frac{1}{2\kappa}. \quad (51)$$

Eqs. (49) and (50) tells that our LSDF's are indeed hybrids of the Wigner-Dyson-like [ $P_\beta(s) \sim s^\beta$  for  $s$  small] and the Poisson-like distributions [ $P_\beta(s) \sim e^{-\kappa s}$  for  $s$  large]. In Figs. 2–4 we exhibit plots of the LSDF's  $P_\beta(s)$  for  $\beta = 1, 2, 4$  and for various  $a$  such that  $e^{-\pi^2/a} \ll 1$ , obtained by numerically solving Eq. (43).

#### IV. ANDERSON HAMILTONIANS AT MIT

In this section we make comparison between the LSDF's and the level number variance in the exact diagonalization of the AH's and our analytic results from multifractal RME's.

As numerical data to compare with, we adopt Ref. [23] for the AH [Eq. (1)] ( $\beta = 1$ ), Ref. [24] for the AH under a magnetic field (5) with  $\alpha = 1/5$  ( $\beta = 2$ ), and Ref. [25] for the AH with spin-orbit coupling (6) with  $\theta = \pi/6$  ( $\beta = 4$ ), at their MIT points. We choose the best fit values of  $a$  from the exponential decay rates  $\kappa$  of the numerical data using Fig. 1. Based on the numerical results  $\kappa = 1.9, 1.8, 1.7$  for  $\beta = 1, 2, 4$ , respectively, we estimate the parameter  $a$  in the potentials of RME's to be

$a = 2.95, 3.55, 3.90$ . Preference could alternately be put on best matchings in the smaller values of  $s$  ( $\lesssim 2$ ), which would lead to  $a = 3.2$  for  $\beta = 1$  [although the difference in  $P_1(s)$  between  $a = 2.95$  and  $a = 3.2$  is tiny]. In Figs. 5–7 we exhibit linear and logarithmic plots of LSDF's of the RME's and the AH's. The numerical data fit excellently with our analytic result from the kernel (14), for a large energy range  $0 \leq s \lesssim 6$  where the LSDF's vary by four to five orders of magnitude. The use of this approximated kernel is justifiable because  $e^{-\pi^2/a} \ll 1$  holds for these values of  $a$ . Small systematic deviations can be attributed to the errors involved in determining the values of  $a$  from the decay rates of numerical LSDF's, and possibly to an essential difference of order  $O(e^{-\pi^2/a})$  between the RME's and the AH's.

Furthermore, we exhibit in Fig. 8 the number variance  $\Sigma^2(S)$  of the orthogonal AH obtained in Ref. [16], together with the RME result (22) with ( $\beta = 1$ )

$$Y_2(x) = K(x)^2 + K'(x) \int_x^\infty K(y)dy \quad (52)$$

at  $a = 3.2$ . We can confirm that not only the asymptotic slopes  $\chi$  of  $\Sigma^2(S)$  (first pointed out by Canali [34], who computed  $\chi$  by the Monte Carlo simulation of RME's), but their full functional forms are in a good agreement for  $L \lesssim 10$ . To recapitulate, we have the following three distinct functional observables (consisting of the correlation functions in the second column) that agree well between the critical AH's and the deformed RME's:

Quantity	Correlation function
Potential	$V(\lambda)$
Number variance	$\Sigma^2(S)$
Level spacing	$P(s)$

In addition, both the critical AH's [9] and the deformed RME's [42] are shown to have multifractal eigenstates, although the sequences of the multifractal dimensions are yet to be compared. Agreements in the unfolded quantities should not be considered a tautological consequence of the first line; one should recall that an identical semicircle spectrum could as well be obtained either from invariant RME's with Gaussian potentials (obeying the Wigner-Dyson statistics), or from diagonal random matrices whose entries are independently derived from the

semicircle distribution (obeying the Poisson statistics), or from any intermediate ensembles. From these grounds, we conclude that the interaction between *unfolded* energy levels of the 3D AH on equilateral ( $L_x = L_y = L_z$ ) toroidal lattices at the MIT is very well described by the form  $|e^{2ax} - e^{2ax'}|^\beta$ , which is common to the RME's with log-squared potentials (9), in contrast to the standard form  $|x - x'|^\beta$  of the Gaussian RME's and the AH's in the metallic regime. We surmise that the dimensionality and the fractal dimensionality enter the critical spectral statistics primarily through a single parameter  $a$ , as long as the multifractality of the critical wave functions is not too strong. Further work is needed to explain this form of the level repulsion from the multifractality (3) of the wave functions, and its origin from microscopic models.

Finally, remarks related to novel numerical results on critical AH's are in order. Recently it was observed that the critical LSDF of the 3D AH is sensitive to the geometry of the lattice, i.e., the topology (boundary condition) [51,52] and the aspect ratio [53], due to the coherence of the critical wave functions maintained over the whole lattice. Since RME's treat randomness on all sites and bonds on equal footing, it is likely that our RME's describe best the critical AH's on maximally symmetric lattices, i.e., equilateral tori, but not those on less symmetric lattices, such as unequilateral toroidal lattices or lattices with boundaries. Besides, since the validity of our expressions for the LSDF's is limited to the case of weak multifractality (relatively small  $a$ ), it will not properly describe the critical orthogonal AH in four dimensions [54], where the level compressibility was observed to be larger than the value in three dimensions ( $\chi \approx 0.27$  [22]) and close to its upper bound  $\chi = 0.5$ .

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## APPENDIX A: FREDHOLM DETERMINANT IN RANDOM MATRIX THEORY

In the Appendix we collect known results on random matrix theories that are relevant to our purpose of evaluating the LSDF of three symmetry classes of RME's. We follow Mehta's classical book [3] and the works by Tracy and Widom [47,55,56]. Readers are referred to them for

detailed proofs. Subsequently we shall concentrate on the case where the spectral correlation is translationally invariant after unfolding.

The joint probability densities of eigenvalues of  $N \times N$  random real symmetric ( $\beta = 1$ ), complex Hermitian ( $\beta = 2$ ), and quaternion self-dual ( $\beta = 4$ ) matrices are given by

$$\begin{aligned}\mathcal{P}_\beta(x_1, \dots, x_N) &= \text{const} \times \prod_{i=1}^N w_\beta(x_i) \prod_{1 \leq i < j \leq N} |x_i - x_j|^\beta, \\ w_1(x) &= e^{-V(x)/2}, \quad w_{2,4}(x) = e^{-V(x)}.\end{aligned}\quad (\text{A1})$$

We use the above convention between the weight functions and the potentials so as to simplify the relations between kernels [Eq. (A5) below]. We introduce the “wave functions”  $\{\psi_i(x)\}_{i=0,1,\dots}$  by orthonormalizing the sequence  $\{x^i e^{-V(x)/2}\}$ , and the projection operator  $K$  to the subspace spanned by the first  $N$  wave functions. As an integration operator acting on the Hilbert space spanned by the wave functions,  $K$  is associated with the kernel (we shall use the same letter for an operator and the kernel associated with it),

$$K(x, y) = \sum_{i=0}^{N-1} \psi_i(x) \psi_i(y). \quad (\text{A2})$$

Then the joint probability densities are expressed in terms of determinants of the kernels [3]:

$$\mathcal{P}_\beta(x_1, \dots, x_N) = \det_{1 \leq i,j \leq N} K_\beta(x_i, x_j), \quad (\text{A3})$$

$$K_2(x, y) = K(x, y), \quad (\text{A4a})$$

$$K_1(x, y) = \begin{pmatrix} S_1(x, y) & S_1 D(x, y) \\ \epsilon S_1(x, y) - \epsilon(x, y) & S_1(y, x) \end{pmatrix}, \quad (\text{A4b})$$

$$K_4(x, y) = \begin{pmatrix} S_4(2x, 2y) & S_4 D(2x, 2y) \\ \epsilon S_4(2x, 2y) & S_4(2y, 2x) \end{pmatrix}. \quad (\text{A4c})$$

Here  $\det$  is to be interpreted as a quaternion determinant in the case of  $\beta = 1$  and 4 [3].  $D$  stands for the differentiation operator, and  $\epsilon$ ,  $S_1$  and  $S_4$  stand for integration operators with kernels [56]:

$$\epsilon(x, y) = \frac{1}{2} \text{sgn}(x - y),$$

$$S_1(x, y) = [1 - (1 - K)\epsilon K D]^{-1} K(y, x), \quad (\text{A5a})$$

$$S_4(x, y) = [1 - (1 - K)DK\epsilon]^{-1} K(x, y). \quad (\text{A5b})$$

A composite operator such as  $\epsilon S_1$  is defined to have a convoluted kernel,  $\epsilon S_1(x, y) = \int_{-\infty}^{\infty} dz \epsilon(x, z) S_1(z, y)$  and so forth, and  $[\dots]^{-1}$  stands for an inverse operator.

The probability  $E_\beta[J]$  of finding no eigenvalues in a set of intervals  $J$  is defined as

$$E_\beta[J] = \int_{x_i \notin J} dx_1 \cdots dx_N \mathcal{P}_\beta(x_1, \dots, x_N). \quad (\text{A6})$$

By virtue of Eq. (A3) and the identity  $\sum_{\{n_i\}} \det M_{n_i n_j} \propto \det M_{nm}$ , it is expressed in terms of the Fredholm determinant of the scalar or matrix kernel [55]:

$$E_2[J] = \det(1 - K_2|_J), \quad (\text{A7a})$$

$$E_{1,4}[J] = \sqrt{\det(1 - K_{1,4}|_J)}, \quad (\text{A7b})$$

where  $|_J$  represents restriction of the kernel to the interval  $J$ .

In the following we assume that the scalar (unitary) kernel  $K$  is translationally invariant and symmetric (the latter property is respected for invariant RME's by construction (A2), but it is violated for RME's with partly deterministic matrix elements [50]),

$$K(x, y) = K(y, x) = K(x - y). \quad (\text{A8})$$

If  $K$  has these two properties, Eqs. (A5) immediately reduce to

$$S_1(x, y) = S_4(x, y) = K(x - y), \quad (\text{A9})$$

because of the relations  $DK = KD$  and  $\epsilon D = 1$ , and the orthogonality of the two projection operators,  $(1 - K)K = 0$ . We assume that  $\lim_{N \rightarrow \infty}$  and the algebraic manipulation that lead to the relation (A5) can be interchanged. In the following we let the notation  $K$  represent its restriction to  $J$ , formerly denoted as  $K|_J$ . If  $J$  consists of a single interval  $[-t, t]$ , we can simplify  $E_\beta[J]$  significantly [47]. To do so, we introduce the resolvent operator  $R = K(1 - K)^{-1}$ , and denote the associated kernel in the form of a matrix element,

$$R(x, y) \equiv \left\langle x \left| \frac{K}{1 - K} \right| y \right\rangle. \quad (\text{A10})$$

Due to the property (A8) assumed on the kernel, it satisfies

$$R(x, y) = R(y, x) = R(-x, -y). \quad (\text{A11})$$

Using this resolvent kernel, the Fredholm determinants (A7) are expressed as

$$E_2[-t, t] = \exp \left\{ -2 \int_0^t dt R(t, t) \right\}, \quad (\text{A12a})$$

$$E_1[-t, t] = \exp \left\{ - \int_0^t dt [R(t, t) + R(-t, t)] \right\}, \quad (\text{A12b})$$

$$\begin{aligned} E_4[-t, t] &= \frac{1}{2} \left( \exp \left\{ - \int_0^{2t} dt [R(t, t) + R(-t, t)] \right\} \right. \\ &\quad \left. + \exp \left\{ - \int_0^{2t} dt [R(t, t) - R(-t, t)] \right\} \right). \end{aligned} \quad (\text{A12c})$$

Equation (A12a) can be proven by taking the logarithmic derivative of Eq. (A7a):

$$\begin{aligned} \frac{d}{dt} \ln E_2[-t, t] &= \text{tr} \left( \frac{1}{1 - K} \frac{dK}{dt} \right) \\ &= -\text{tr} \left( \frac{1}{1 - K} K (-t) \langle -t | + |t \rangle \langle t | \right) \\ &= -2 \left\langle t \left| \frac{K}{1 - K} \right| t \right\rangle. \end{aligned} \quad (\text{A13})$$

Eqs. (A12b,c) can be proven analogously from Eqs. (A4b), (A4c), and (A7b). These relations are equivalent to Eqs. (6.5.19) and (10.7.5) of Ref. [3] because  $\exp\{-\int_0^t dt [R(t, t) \pm R(-t, t)]\}$  is a Fredholm determinant of the kernel  $K(x, y) \pm K(-x, y)$  (although Ref. [3] concerns primarily the sine kernel, the proofs of these equations are equally valid for any translationally invariant and symmetric kernel).

Now we set  $2t = s$  and denote  $E_\beta(s) = E_\beta[-s/2, s/2]$ . The probability  $P_\beta(s)$  for a pair of consecutive eigenvalues to have a spacing  $s$  is clearly equal to the probability of finding an eigenvalue in an infinitesimal interval  $[-s/2 - \epsilon, s/2]$ , another in  $[s/2, s/2 + \epsilon']$  and none in between  $[-s/2, s/2]$ , divided by  $\epsilon \epsilon'$ . Thus we have

$$P_\beta(s) = E_\beta''(s). \quad (\text{A14})$$

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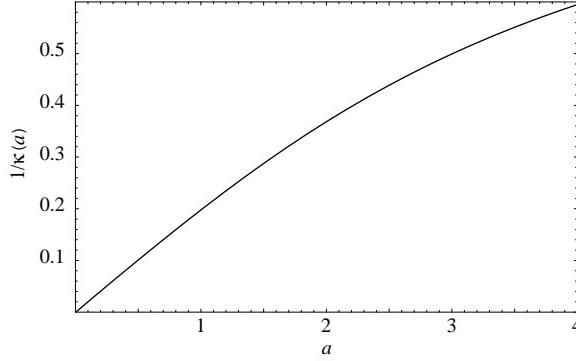


FIG. 1. The decay rate  $\kappa(a) = R_a(\infty)$  of the LSDF.

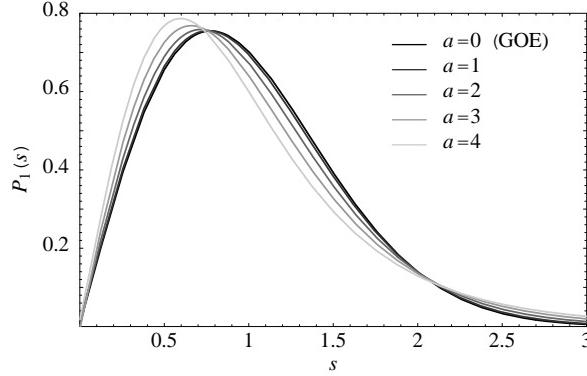


FIG. 2. The LSDF  $P_1(s)$  of the orthogonal ensemble with the kernel (14).

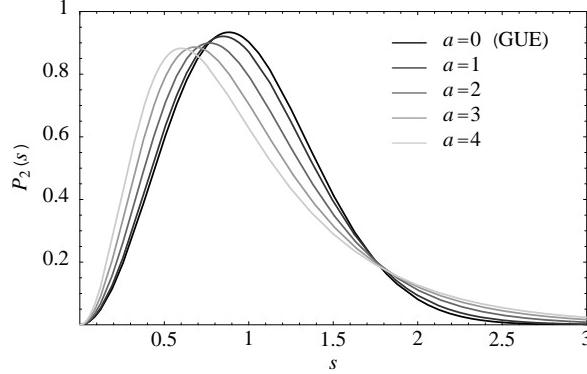


FIG. 3. The LSDF  $P_2(s)$  of the unitary ensemble with the kernel (14).

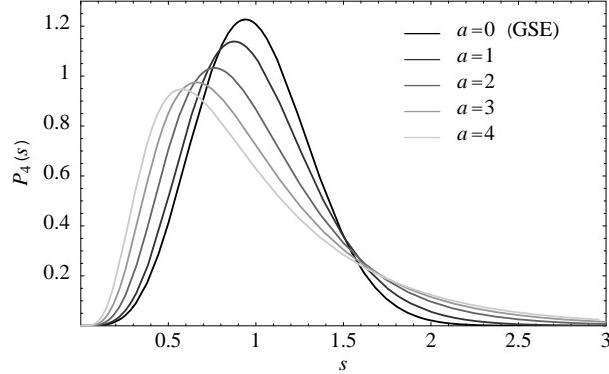


FIG. 4. The LSDF  $P_4(s)$  of the symplectic ensemble with the kernel (14).

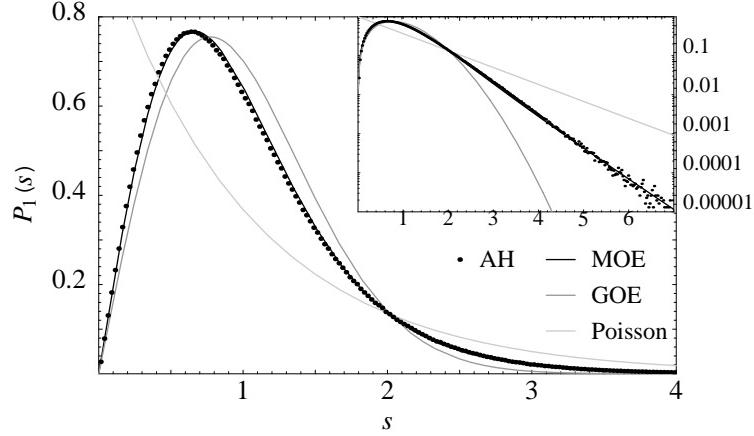


FIG. 5. The LSDF's  $P_1(s)$  of the multifractal orthogonal ensemble (MOE) at  $a = 2.95$  and of the Anderson Hamiltonian (1) at the MIT point  $W = 16.4$ , on a lattice of size  $L^3 = 12^3$ . Numerical data are reprinted from Fig. 1 in Ref. [23] courtesy of Zharekeshev.

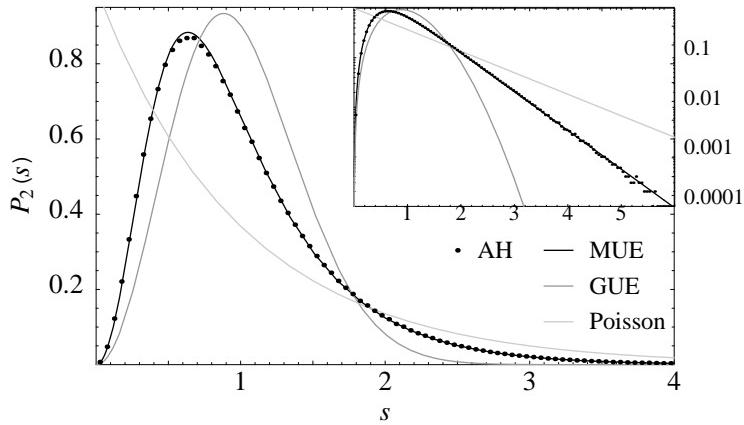


FIG. 6. The LSDF's  $P_2(s)$  of the multifractal unitary ensemble (MUE) at  $a = 3.55$  and of the AH (5) under a magnetic field  $\alpha = 1/5$  at the MIT point  $W = 18.1$ , on a lattice of size  $L^3 = 5^3$ . Numerical data are reprinted from Fig. 1 in Ref. [24] courtesy of Schweitzer.

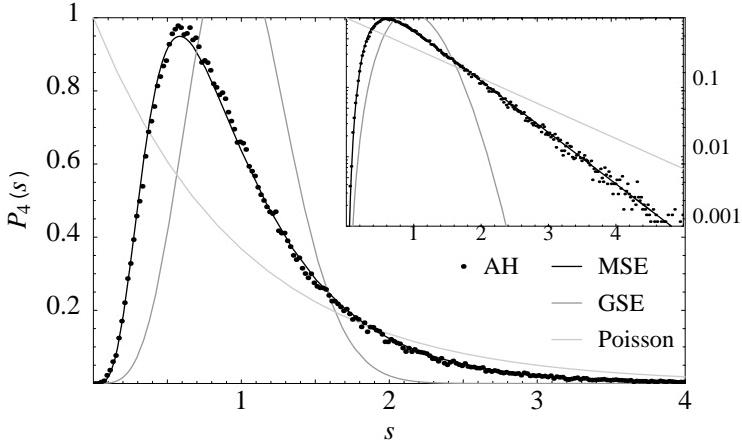


FIG. 7. The LSDF's  $P_4(s)$  of the multifractal symplectic ensemble (MSE) at  $a = 3.90$  and of the AH (6) with spin-orbit coupling  $\theta = \pi/6$  at the MIT point  $W = 19$ , on a lattice of size  $L^3 = 12^3$ . Numerical data are reprinted from Figs. 2 and 3 in Ref. [25] courtesy of Kawarabayashi.

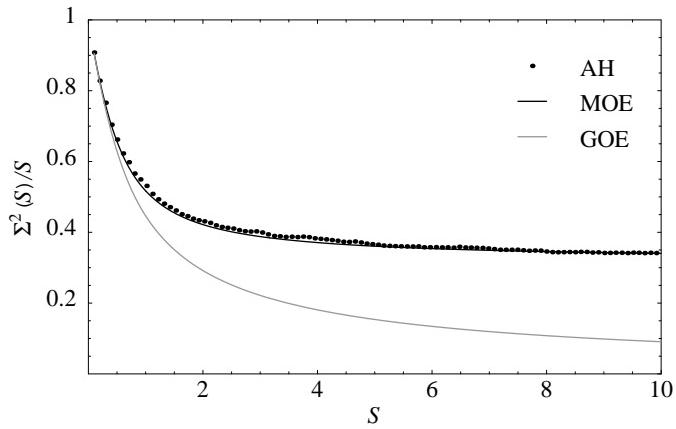


FIG. 8. The level number variance  $\Sigma^2(S)$  (divided by  $S$ ) of the multifractal orthogonal ensemble at  $a = 3.2$  and of the AH (1) at the MIT point  $W = 16.5$ , on a lattice of size  $L^3 = 10^3$ . The Poisson distribution corresponds to  $\Sigma^2(S)/S = 1$ . Numerical data are reprinted from Fig. 2 (b) in Ref. [16] courtesy of Evangelou.